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Interatomic potentials and the simulation of lattice defects in metals.

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effect A (helium, vacancy) from a
filled with n helium atoms
A (helium atom or vacancy) in a
filled with n helium atoms
m atom in a dislocation core filled
m atom in the core of a dislocation
atoms present in the core at some
om considered.

SUMMARY

The computer simulation technique is applied to investigate the properties of point defects and line defects in metals. For that purpose crystallites are constructed in which these defects are simulated. In the case of line defects (dislocations) the initial positions of the atoms, surrounding the dislocations, are determined using the elastic theory of anisotropic media (chapter 2). Hereafter the atoms in such crystallites are allowed to relax to their minimum potential energy positions under the influence of the interatomic forces. These forces are derived from interatomic interaction potentials. These potentials are together with the boundary conditions of the simulated crystallite the main input data in these computer simulation models.

In chapter 3 extensive attention is paid to the interactions between the atoms in a crystal lattice. Main information on the interatomic forces and the derivatives of these forces can be obtained from the experimental phonon dispersion curves and elastic constants. The latter physical data, which have been used by various authors in potentials proposed, give a more limited insight than the former. In this chapter therefore, potentials are presented which have been fitted to the experimental phonon dispersion curves and the formation energy of a vacancy. Such potentials, however, are not unique. Additional information on certain interval of the potentials is necessary. In this chapter also a method is presented to include the migration on certain intervals of the potentials is necessary. For that purpose in this chapter a method is presented to include the migration energy as an additional fitting constant. Using such potentials for bcc metals (Cr, Mo, Fe, W, Ta) and fcc metals (Pd, Ni, Cu, Ag, Au) some properties of point defects are calculated.

For molybdenum and copper the atomic configurations of edge and screw dislocations are investigated (chapter 4). The results, obtained in the computer simulation model (atomistic model), are compared with those obtained using the elastic theory of anisotropic media. Also the influence of the potentials used is studied. Special attention is paid to the dissociation of both the edge and screw dislocations into partial

dislocations. This phenomenon has been observed in our calculations for copper.

In chapter 5 the interaction between helium atoms and both point defects and dislocations is investigated. For that purpose, interaction potentials are derived describing the interaction between two helium atoms and potentials describing the interaction between a helium atom and a metal atom. These potentials are fitted to the activation energies of helium desorption from vacancies filled with helium atoms as experimentally measured in helium desorption experiments. Using these potentials the interaction of helium atoms with vacancies and with edge and screw dislocations in molybdenum is studied. For comparison the calculations have been repeated using potentials quoted in the literature. The results of the atomistic calculations are compared with the results obtained using the elastic theory.

SAMENVATTING

De computersimulatietechniek wordt gebruikt om de interactie tussen punt- en lijnfouten te onderzoeken. In hoofdstuk 2 wordt een model ontwikkeld waarin deze fouten (dislocaties) worden beschreven. Deze dislocaties worden bepaald met behulp van de anisotrope media (hoofdstuk 2). De fouten worden vervolgens losgelaten en de energieën worden berekend waarvoor hun potentiële energieën worden berekend. De resultaten vinden plaats onder invloed van de interatomaire interacties. De resultaten worden samen met de randvoorwaarden vergeleken met de belangrijkste invoergegevens.

In hoofdstuk 3 wordt uitgegaan van de wisselwerking van atomen in een medium. De interatomaire krachten en de elasticiteitsconstanten worden afgeleid uit experimenteel gemiddelde elasticiteitsconstanten. Laatstgenoemde diverse auteurs in hun potentiaalenergieën. Het geeft een beperkter inzicht dan eerstgenoemde ook potentialen voorgesteld, die krommen en aan de vormingsenergieën. De potentialen zijn echter niet uitsluitend intervallen van de potentialen. Om de potentialen aan te passen, zoals die experimenteel wordt gevonden, die voor zowel k.r.g. metalen (Ni, Pd, Cu, Ag, Au) zijn opgesteld. De puntfouten (vacatures en interstitieel atomen) worden beschreven.

Voor de metalen molybdeen worden rand- en schroefdislocaties onderzocht met een computersimulatiemodel (atomistisch model). De resultaten verkregen met de elasticiteitstheorie. Ook de invloed van de gebruikte